Quasi-continuum approximation to the Nonlinear Schrödinger equation with Long-range dispersions

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(Dated: February 8, 2008)

The long-wavelength, weak-dispersion limit of the discrete nonlinear Schrödinger equation with long-range dispersion is analytically considered. This continuum approximation is carried out irrespective of the dispersion range and hence can be assumed exact in the weak dispersion regime. For nonlinear Schrödinger equations showing finite dispersion extents, the long-range parameter is still a relevant control parameter allowing to tune the dispersion from short-range to long-range regimes with respect to the dispersion extent. The long-range Kac-Baker potential becomes unappropriate in this context owing to an "edge anomaly" consisting of vanishing maximum dispersion frequency and group velocity(and in turn soliton width) in the "Debye" limit. An improved Kac-Baker potential is then considered which gives rise to a non-zero maximum frequency, and allows for soliton excitations with finite widths in the nonlinear Schrödinger system subjected to the long-range but finite-extent dispersion.

PACS numbers: 03.50.-z, 42.65.Tg, 45.20.-d

Considerable efforts have been devoted to understanding physics of one-dimensional($1D$) systems in which dynamical properties are dominated by the competition between nonlinearity and dispersion. The Nonlinear Schrödinger equation(NLSE) is one of most investigated nonlinear equations in these contexts, and widespread applications can be found in various fields of condensed matter physics. Very recently, a new path was opened in the interest to this equation toward materials with long-range(LR) dispersions [1, 2]. These LR dispersions are thought to occur in two different kinds namely, intrachain dispersions involving long-range interactions among particles of a single discrete chain [1], and interchain dispersions related to the couplings between several $1D$ chains with short-range interactions [2]. Each of these two kinds of LR dispersion deserves interest since both lead to two distinct but real physical contexts. Magnetic spin chains and Davydov's molecular chains [3, 4] are two examples of natural systems in which the first kind of LR dispersion arises. As for the second, we strongly suspect it may provide an excellent way to model systems made of several weakly coupled $1D$ chains. Indeed, if the coupling between the $1D$ chains is not too strong the model can stand as a good approximation of a quasi-one-dimensional($Q1D$) material. To this viewpoint, we expect the second kind of LR dispersion to find direct applications in nonlinear optics or Bose-Einstein condensate(BEC) systems [11, 12] where soliton compression phenomena [5, 6, 7] are likely to occur, e.g. resulting from periodic arrangements of dielectric elements as in photonic crystals [8, 9, 10] or from the configuration of an optically coupled array of BEC lattices.

The present work deals with the first kind of LR dispersion. The discrete NLSE in this cas writes [1]:

$$-i\psi_{nt} + \sum_{m\neq n}^{L} J_{m-n}(\psi_m - \psi_n) + g \mid \psi_n \mid^2 \psi_n = 0. \quad (1)$$

where ψ is the complex wavefunction, g is a nonlinear coupling(hereafter assumed positive) and J_{m-n} is the potential creating the LR dispersion. Equation (1) has been discussed by few authors [1] assuming exponential and power-law LR potentials. These works focus on soliton solutions as well as on their stability and suggest rich physical properties related to the LR dispersion. In particular, authors of ref. [1] combined lattice discreteness and LR dispersion and showed that different soliton regimes may be stabilized from the interplay of these two factors. In connection with the variety of stability regimes, the authors suggested a switching mechanism by which the transition between different bistable localized states could be monitored by tuning parameters of the LR potential. In biophysical systems where inter molecular interactions often display great sensitivity to the flexibility of molecular backbones, such a switching mechanism is likely to be due to the "contraction-relaxation" features of bond danglings. In this view, provided the bond length is commensurate with the wavelength of intra molecular excitations, the discrete NLSE with LR dispersion(LRNLSE) is indeed a good approximation for nonlinear molecular vibrations and nonlinear molecular excitons can well be understood as highly discrete and localized solutions of this equation with relatively narrow shapes(compared with the lattice constant). However, if the bond length is short and the molecular masses large, narrow excitons are less probable since long-wavelength processes will tend to dominate. This last situation is the commonly studied one in magnetic spin chains and Davydov models in the short-range dispersion regime. The associate NLSE admits single pulse and dark soliton solutions in the continuum limit. Strictly speak-

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ing, the continuum short-range NLSE(SRNLSE) is the long-wavelength and weak-dispersion limit of the discrete SRNLSE [13].

The goal of the present study is to point out that an equivalent limit is also accessible for the discrete LRNLSE irrespective of the range of lattice dispersion. For this purpose, we will follow a Fourier transform method consisting to first construct the dispersion function of the LR system, and next extract the continuum NLSE from a second-order expansion of the dispersion function. As this expansion does not involves some constraint on the range of lattice dispersion, the continuum LRNLSE derived from our long-wavelength and weak-dispersion approximation is indeed an exact equivalent of the celebrated continuum SRNLSE. Our interest to the problem was motivated after noting that the dispersion curves of the NLSE with exponential LR potentials always displayed the linear shape at small wavectors, and that only their slopes were affected by the variation of the LR parameter. In this context, no physical or mathematical constraint prevents us from linearizing the dispersion relation of the LRNLSE so far as the long-wavelength limit is concerned. Actually, the variation of the slope of the dispersion curve with varying dispersion range is the signature of a varying sound speed. That the entire effect of the LR dispersion is confined on the sound speed agrees quite well with the spirit of weak-dispersion approximations. Disorder, whcih is another interesting source of residual dispersion, often causes the same effect. We would also like to draw attention on similarity between the current problem and that discussed by Konotop [14] in terms of the group velocity of a discrete nonlinear monoatomic lattice with Kac-Baker(KB) [15, 16] LR interaction.

For illustrative purpose, we will assume two different LR potentials one of which is the KB potential i.e.($\ell = m - n$):

$$J_{KB}(\ell) = J_o\frac{1-r}{2r}r^{|\ell|}, \quad 0 \le r < 1, \tag{2}$$

The second LR(MKB) potential is defined as:

$$J_{MKB}(\ell) = J_o\frac{1-r}{2r(1-r^L)}r^{|\ell|}, \quad 0 \le r \le 1 \tag{3}$$

In both (2) and (3), J_o is the potential constant, r is the LR parameter and L is half of the spatial extent of the LR dispersion. Indeed, we suppose the actual distance on which LR dispersions effectively spread out is not absolutely equal to the total size of the spin or molecular system. For instance we can think of an infinite-size system undergoing finite-extent dispersions as it really happens in most cases. Neverthess, to avoid losing track of the usual necessary constraints on LR dispersion potentials it is needful to mathematically probe the validity of such possibility. For this purpose we sum J_{m-n} over L obtaining:

$$\begin{aligned}\sum_{\ell=-L}^{L} J_{KB}(\ell) &= Jo(1-r^L),\\ \sum_{\ell=-L}^{L} J_{MKB}(\ell) &= Jo.\end{aligned} \tag{4}$$

As one sees, the norm of the KB potential is length dependent and becomes constant only in the "thermodynamic" limit. The dependence of the total amplitude of the KB potential on L, which we term "edge anomaly" [17], is the main motivation of our interest to the MKB potential. Of course, this edge anomaly does not shades at all the rich physics behind the KB model though seeming to restrict its validity to infinite-length materials and systems with infinite dispersion extents. Still, making the potential amplitude a function of L as in the MKB potential can turn into a relevant advantage for NLSEs with finite dispersion extents. In this case the potential amplitude can be adjusted to a desired dispersion extent regardless of whether the total length of the system is finite or not. To this point, note that J_{MKB} reduces to J_o in the short-range limit(i.e. $L = 1$) irrespective of the value of r. On the contrary, for J_{KB} we need to set $r = 0$. Below a finite-length solution of the continuum LRNLSE will be derived and will appear to be a periodic function, the period of which can be set equal to L. Doing so, we confine solitonic excitations on the effective spatial interval spread by the dispersion. Since the LR paramater r allows monitoring the strength of the dispersion regardless of its extent, the theory will still be valid whether the system is of finite size or not.

As we are interested with the nonlinear localized solution of eq. (1), we can write down the wavefunction $\psi_n(t)$ as follow:

$$\psi_n(t) = \phi_n \, exp(-i\nu t). \tag{5}$$

Inserting (5) in (1) we obtain:

$$-\nu\phi_n + \sum_{m\neq n}^{L} J_{m-n}(\phi_m - \phi_n) + g\phi_n^3 = 0. \tag{6}$$

Since the new wavefunction is only space dependent, (6) is a discrete nonlinear static equation and a spatial Fourier transform can be performed. We define the Fourier transform(per unit length) of ϕ_n as:

$$\phi_n = \int dq \, \phi_q \, e^{-iqnd}, \tag{7}$$

where d is the lattice spacing and q the wavector. Except the LR potential, all coefficients in eq. (6) are constant so their Fourier transforms are single inegrals. Remark that the nonlinear term of this equation describes an isotropic "three-mode" coupling and as consequence the associate Fourier tranform will be a simple integration

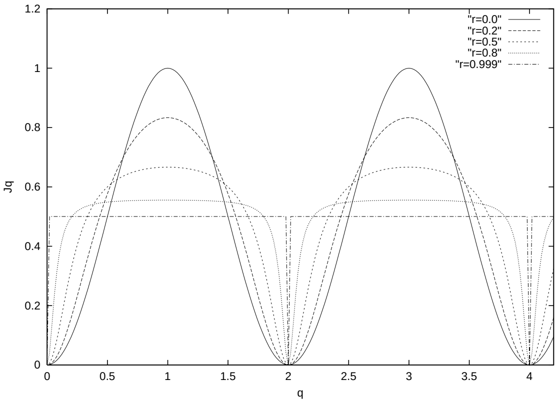

FIG. 1: Plot of the dispersion function versus q(in the reduced unit q/π) for some values of the long-range parameter r. Here the extent of dispersion is taken infinite.

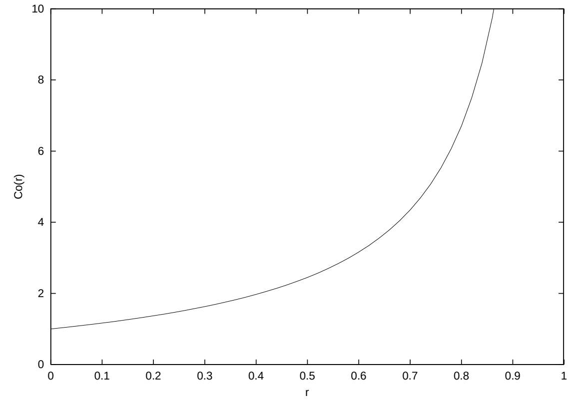

FIG. 2: Plot of the sound speed versus r for the NLSE with infinite dispersion extent.

over the single wavector common to the three coupled fields. The most interesting part of the discrete nonlinear static equation is thus the second term whose Fourier tranform writes:

$$\begin{aligned} \sum_{m\neq n}^{\infty} J_{m-n}(\phi_m - \phi_n) &= -\int dq\, J_q(r)\,\phi_q\, e^{-iqnd}, \\ J_q(q) &= J(r)\sum_{\ell=1}^{L} r^{\ell}\left[1-\cos(q\ell d)\right], \end{aligned} \tag{8}$$

where $J(r)$ can assume two distinct forms in connection with (2) and (3) i.e.:

$$\begin{aligned} J_{KB}(r) &= J_o\frac{1-r}{r}, \\ J_{MKB}(r) &= J_o\frac{1-r}{r(1-r^L)}. \end{aligned} \tag{9}$$

The quantity $J_q(r)$ is the function governing the spatial dispersion of the LRNLSE. The sum appearing in this function is restricted to L. However, it can be extended to infinity provided the chain length also is infinite. Since this last context is more familiar, let us first examine the case $L \to \infty$. On fig. 1 we plot J_q versus q for some values of r. The just mentioned sum is evaluated numerically for the two LR potentials. According to (3), both potentials reduce to the same expression in the infinite-dispersion limit.

Fig.1 shows that $J_q(r)$ remains a sinusoidal function for the whole interval of values of r, and only slopes of the dispersion curves vary. To check this assertion, a numerical expansion of the dispersion function J_q was carried out up to the second-order term for weak values of $q\,d$. The leading and first-order terms vanish but not the second-order term. The coefficient of this last term is nothing else but the square of the sound speed $C_o(r)$ [14], which is plotted in fig. 2 as a function of the LR parameter r.

An exact analytical expression of $J_q(r)$ for finite L can be obtained using the following identity:

$$\begin{aligned} V_r(q) &= \sum_{\ell=1}^{L} r^{\ell}\cos(qd\ell), \\ &= \frac{r\cos(\tilde{q}) - r^2 - r^{(L+1)}[\cos((L+1)\tilde{q}) - r\cos(L\tilde{q})]}{1-2r\cos(\tilde{q})+r^2}. \end{aligned} \tag{10}$$

and is given by:

$$J_r(q) = J(r)[V_r(0) - V_r(q)], \tag{11}$$

We can check that this analytical expression is fully consistent with numerical curves in fig. 1. To see the effects of finite L on the dispersion of our system, in figs. 3 and 4 we have drawn (11) versus r placing ourselves at the edge of the first Brillouin zone i.e. $q = \pi$, and using $L = 10,\ 20,\ 1000$. We see that the maximum frequency is sensible to the extent of dispersion for the KB potential and not for the MKB potential. However, the two sound speeds(figs. 5 and 6) fill effects of finite values of L but tend to the same limit when L becomes sufficiently large(i.e. infinite). In the case of KB potential, there occur maxima in $C_L(r)$ at $r < 1$ and the sound speed vanishes as $r \to 1$ for finite L. As opposed to this first model, $C_L(r)$ is monotonous in the MKB case and tends to a finite value as $r \to 1$ when L assumes finite values.

The analytical expression of the sound speed plotted in figs 5 and 6 was derived from (11) by an analytical expansion of $J_q(r)$ to the second order for weak values of the product $q\,d$. Since here too the leading and first-order terms vanish, we are only left with the second-order term proportional to q^2. Strictly, this expansion corresponds to a continuum-limit approximation for long-wavelength($nd \to x$) and weak-dispersion ($qd << 1$) excitations. Thus, with regard to the minus sign in front of the right-hand side of the first equation in (8), an inverse Fourier tranform of the q^2 term produces the following

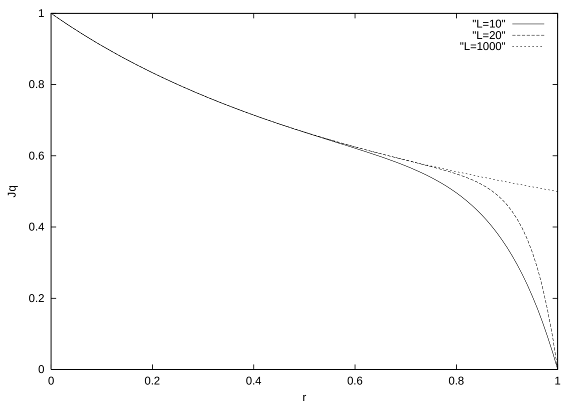

FIG. 3: Dependence of the maximum frequency on the dispersion extent for the LRNLSE with the KB potential.

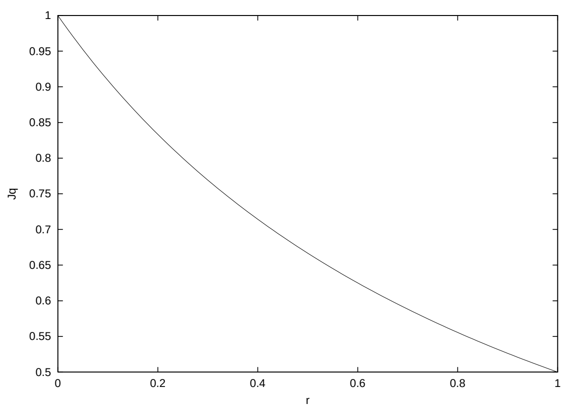

FIG. 4: The maximum frequency of the LRNLSE with the MKB potential. Note the absence of a dependence on the dispersion extent.

continuum nonlinear second-order equation:

$$C_L^2(r)\phi_{xx} - \nu\phi_n + g\phi_n^3 = 0. \tag{12}$$

The square of the sound speed $C_L^2(r)$ is proportional to the second-order derivative of $J_q(r)$ i.e.:

$$C_L^2(r) = (1/2)\partial_{qq}\Omega^2(q)|_{q\to 0}. \tag{13}$$

It is useful to note that the discrete LRNLSE (1) itself could be treated in a similar manner and would lead to the usual form of continuum NLSE.

For positive values of g and ν, equation (12) admits finite-length soliton solutions [18] given in terms of Jacobi Elliptic functions [19]:

$$\begin{aligned}\phi(x) &= \phi_o cn\left(\frac{x}{\ell_o}|\kappa\right), \qquad \kappa \geq 1,\\ \phi_o &= \sqrt{\frac{2\kappa^2}{2\kappa^2-1}}\left(\frac{\nu}{g}\right)^{1/2}, \qquad \ell_o^2 = \frac{C_L^2(r)}{\nu}(2\kappa^2-1).\end{aligned} \tag{14}$$

cn, which is the Jacobi Elliptic function, is periodic in x with a period $L_o = 4\ell_o K$ where K is the complete Elliptic

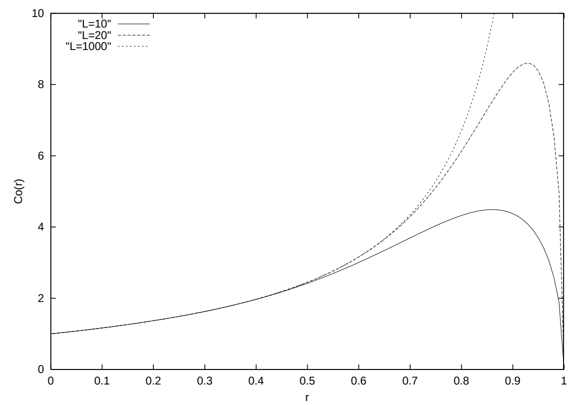

FIG. 5: Dependence of the sound speed on the dispersion extent for the KB potential.

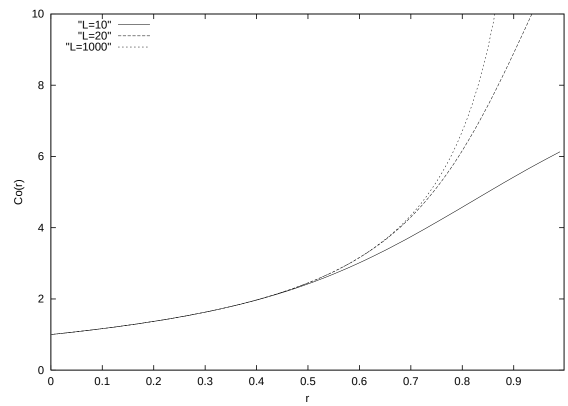

FIG. 6: Dependence of the sound speed on the dispersion extent for the MKB potential.

integral of the first kind. In general, cnoidal waves provide adequate representations of the soliton solutions of finite-length systems in connection with the finite magnitude of L_o. In this viewpoint, we can decide to set $L = L_o$ which amounts to confine all solitonic excitations within the interval spread by the LR dispersion. In the limit $\kappa = 1$, (14) turns to the single-pulse soliton:

$$\begin{aligned}\phi(x) &= \phi_o sech\left(\frac{x}{\ell_o}\right)\\ \phi_o &= \sqrt{\frac{2\nu}{g}}, \qquad \ell_o^2 = \frac{C_L^2(r)}{\nu}\end{aligned} \tag{15}$$

and $L_o \to \infty$. However, L can be kept finite in this limit. According to the dependence of ℓ_o on the sound speed, we expect the pulse width to assume behaviours of $C_L(r)$ with respect to the LR parameter r. On fig. 2, $C_\infty(r)$ was an infinitely increasing function of r. This means the pulse width is quickly diverging as $r \to 1$ for infinite dispersion extents. Following the effect of an assumption of finite values of L on the sound speed, finite-width single-pulse solitons are likely to be observed in a NLSE with LR dispersion and corresponds, in a physical context,

to a system in which the extent of dispersion does not follow the system size. However, since the sound speed always goes to zero as $r \to 1$ for the KB potential, this model is relatively less suitable in such physical contexts as opposed to the apparently advantageous features of the MKB potential.

Acknowledgments

I would like to express thanks to Dr. T. C. Kofané from the University of Yaoundé, cameroon for numerous advices. Part of this work was carried out as the author was guest at the Abdus Salam International Centre for Theoretical Physics Trieste, Italy.

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